On numerical experiments for Cauchy problems of elliptic operators $\stackrel{\diamond}{\approx}$

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Abstract

Over the last decade, there has been a considerable amount of new numerical methods being developed for solving the Cauchy problems of elliptic operators. In this paper, with some new classes of numerical experiments, we re-verify the conclusions in the review article [EABE,31(4):373-385,2007] concerning the effectiveness of solving Cauchy problems with the method of fundamental solutions.

Keywords: Cauchy problem; Method of fundamental solution; Boundary singularity

1. Introduction

Cauchy problems of elliptic operators are typically ill-posed problems whose solutions do not continuously depend on the input Cauchy data. However, these ill-posed problems play important roles in many science and engineering models such as steady-state inverse heat conduction [10], electrocardiology [6], nondestructive testing [11], and so on. For the sake of numerical computations, a small perturbation or error in the input may lead to an enormous error in the numerical solution.

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The Cauchy problem we consider is in the form of

$$\mathcal{L} u = 0, \quad \text{in } \Omega \subset \mathbb{R}^d, \partial_{\nu}^{(k)} u = g_k, \quad \text{on } \Gamma, \, k \in \{0, \, 1\},$$
(1)

where \mathcal{L} is a differential operator of elliptic type, Ω is a bounded simply connected domain in \mathbb{R}^d , $\Gamma \subsetneq \partial \Omega$ is the Cauchy boundary, and $\partial_{\nu}^{(k)}$ is the *k*-th order normal-derivative. The goal here is to determine a distribution function $u \in C^2(\Omega) \cap C^1(\overline{\Omega})$ that satisfies (1) with the provided Cauchy data $g_k, k \in \{0, 1\}.$

2. Redundancy in Cauchy data

For convenience, researchers usually pick exact solutions that satisfy the governing equation $\mathcal{L}u = 0$ in the whole space \mathbb{R}^d in order to generate the Cauchy data $g_k, k \in \{0, 1\}$. This Cauchy data is then used to verify different numerical methods for solving (1). In some situations, this approach may yield overdetermined test problems—the key message we want to deliver in this paper. Although it is not our aim to come up with a general mathematical theory about the redundancy in Cauchy data, below is a specific situation in which the Neumann boundary data is not necessary to guarantee unique solution in the Cauchy problem.

Consider a Cauchy problem of the Laplace operator in two-dimensions for simplicity. Suppose the *exact* Cauchy solution u^* of (1) is harmonic everywhere in \mathbb{R}^2 . For simplicity, let us consider Ω being the unit circle and the Cauchy boundary Γ being the upper half. Since u^* is harmonic and therefore analytic, the Dirichlet data $g_0(\theta), \theta \in I := [0, \pi]$, is real analytic. Now further assume that the Taylor expansion of u^* at the origin has a radius of convergence R > 1. Then the two (1D real) analytic functions, $u^*|_{r=1}(\theta)$ and $g_0(\theta)$, agree on I; by the unique continuation of analytic functions, they also agree on $[-\pi/2, 3\pi/2]$. Having Dirichlet boundary condition on the whole boundary $\partial\Omega$ yields the Dirichlet (forward) problem and (1) has unique solution without the Neumann boundary condition.

Note that in the above situation, having a unique solution does not imply the solution process is stable. The Cauchy problem is still ill-posed and is highly sensitive to any noise in the Cauchy data. We observe that the test problems in some literatures, i.e.

In [5]: $u^* = y^3 - 3yx^2$,

In [9]: $u^* = xy$,

In [16]: $u^* = \exp(0.5x)\sin(0.5y)$ and $u^* = x + y$,

In [17]: $u^* = x^3 - 3xy^2 + \exp(2y)\sin(2x) - \exp(x)\cos(y)$,

In [19]: $u^* = 10y - 9$, and others in [1, 2, 3, 4, 13, 14, 15],

the tested Cauchy problems with globally harmonic solutions may also have numerically redundant Cauchy data.

Numerically, we can sometime solve the Cauchy problem (1) with only one boundary condition on Γ . Figure 1 and 2 show some numerical reconstructions when we apply the MFS directly (without regularization) to solve (1) with Dirichlet data only. We show only a subset of the collocation points in order to keep the figures easily readable. Figures 1(a)-1(b) are the reconstructed solutions in a unit circle and square respectively using Dirichlet data $g_0 = \exp(x) \cos(y) = u^*|_{\Gamma}$ (with $\Delta g_0 = 0$). It can be seen that the numerical solutions closely agrees with the corresponding exact solutions; our argument above (on the unit circle) cannot explain why the latter works on the square domain. While $g_0 = \cos(x) \exp(y)$ (also with $\Delta g_0 = 0$) on half circle is sufficient to solve (1), Figure 2(b) is a typical sign suggesting that the Neumann data is essential for this Cauchy problem on the square domain.

To ensure the conclusions drawn for any numerical method are completed, they should not be all depends on test problems with redundant data. To determine if a test problem may have "numerical" redundancy in data, one can solve the Cauchy problem with noise-free Dirichlet data only as a *patch test for data redundancy*. We aim to identify test problems that cannot be solved without the Neumann data, as seen in Figure 2(b). The rest of this paper is devoted to some test problems that will not suffer from trouble of redundant Cauchy data.

3. Suggested test 1: singularity in $\mathbb{R}^d \setminus \overline{\Omega}$

The easiest and most convenient way is to construct numerical experiments using a function which satisfies the government equation everywhere with singularity in $\mathbb{R}^d \setminus \overline{\Omega}$. Under this setup and with the right geometry, the Cauchy problem can sometimes be solved with one Dirichlet data only. However, the singularity-to-domain distance has a strong influence on the stability and the patch test will fail (i.e. Neumann data becomes essential) if we take the singularity close enough to $\partial\Omega$.



Figure 1: Patch test: $g_0 = \exp(x)\cos(y)$ for data redundancy—Cauchy problems (1) with only one Dirichlet data; — (exact solutions), • (collocation points), and \blacksquare (numerical solutions).



Figure 2: Patch test: $g_0 = \cos(x) \exp(y)$ for data redundancy—Cauchy problems (1) with only one Dirichlet data; — (exact solutions), • (collocation points), and \blacksquare (numerical solutions).

For example, we can take the exact solution of (1) as $u^* = \log((x-a)^2 + (y-b)^2)$ with singularity at $(a, b) \notin \Omega$ and use it to generate the Cauchy data g_0 and g_1 . In Table 1, we show the accuracies of the MFS approximations with various regularization techniques for (a, b) = (2, 0) and (10, 0). Neumann boundary data is necessary for the former; whereas the latter passes the (noise-free) patch test that can be solved without the Neumann data. For the regularization techniques that work (TR or DSVD combined with either LC or GCV as recommended in [17]), they all yield better accuracy¹ in the latter case when the singularity is far away. An appropriate experiment of this type should *not* have a far-away singularity.

(a,b) = (2,0)						
Method	TR-LC	DSVD-LC	TSVD-LC	TR-GCV		
ϵ_{∞}	0.2851	0.2389	25.1520	0.1122		
Method	DSVD-GCV	TSVD-GCV	TR-DP	DSVD-DP		
ϵ_{∞}	0.1002	41.6994	25.4118	11.8107		
		(a,b) = (10,0)				
Method	TR-LC	(a,b) = (10,0) DSVD-LC	TSVD-LC	TR-GCV		
$\begin{array}{c} \\ \text{Method} \\ \hline \epsilon_{\infty} \end{array}$	TR-LC 0.0258	(a,b) = (10,0) DSVD-LC 0.0424	TSVD-LC 66.9753	TR-GCV 0.0085		
$\begin{tabular}{c} Method \\ \hline ϵ_{∞} \\ Method \end{tabular}$	TR-LC 0.0258 DSVD-GCV	(a, b) = (10, 0) DSVD-LC 0.0424 TSVD-GCV	TSVD-LC 66.9753 TR-DP	TR-GCV 0.0085 DSVD-DP		

Table 1: Exact solution with singularity. The maximum errors with various regularization methods under 1% noise.

4. Suggested test 2: $u|_{\partial\Omega} \rightarrow g_1$

A more practical situation is to pick some *nonharmonic* function (i.e. does not satisfy government equation everywhere) to generate the Cauchy data g_0 in closed form. If we take g_0 as the Dirichlet boundary condition of the whole boundary $\partial\Omega$, we have a direct problem of the elliptic type. Since the data-generating function is nonharmonic, the comments in [8, 18] suggest that we should not expect the MFS approximation to be of machine-epsilon accuracy. Optimizing the MFS for direct problems is out of the scope of

¹Maximums norms of $\log((x-a)^2 + (y-b)^2)$ are 2.3026 and 4.8040 for (a,b) = (2,0) and (10,0), respectively.

this paper; we refer readers to the original articles for details. The rule of thumb is that as long as g_0 is smooth on the boundary, the MFS should be able to do its job correctly and provide us the solution of the direct problem with relatively high accuracy. For the Laplace operator, we can always verify the accuracy with the maximum principle. Once we have an approximate solution in hand, we can numerically evaluate its normal derivative on the Cauchy boundary Γ . It is easily doable if we employ the MFS to solve the direct problem; all we have to do is to differentiate the basis functions (that is the fundamental solutions).

We take $g_0 = x^2 y^3 = u^*|_{\partial\Omega}$ in this demonstration. First, we solve the Laplace equation with Dirichlet boundary condition $u|_{\partial\Omega} = g_0$ to obtain a numerical approximation u_n with ϵ_{∞} is 7.6258e-012. Then, we determine the other Cauchy data by $g_1 = u_{\nu}|_{\Gamma}$. All Cauchy data needed for the inverse problem (1) are now available. One important note to mention before we start solving the inverse problem is that the distribution of source points for the direct and inverse parts here should be different in order to avoid the inverse crime. That is, (nearly) the same theoretical ingredients are employed to synthesize as well as to invert data in an inverse problem. This act has been qualified as trivial and therefore should be avoided [7]. All MFS approaches in [17] are tested with 1% noise. We report the maximum error ϵ_{∞} on boundary and the relative root mean square errors ϵ_2 over the domain in Table 2. We observe that TR-LC and TR-GCV work better than other combinations. The other two techniques, DSVD-LC and DSVD-GCV, recommended in [17], are both working reasonably well here.

Method	TR-LC	DSVD-LC	TSVD-LC	TR-GCV
ϵ_{∞}	0.0015	0.0417	3.7341	0.0015
ϵ_2	0.0044	0.1270	6.1102	0.0044
Method	DSVD-GCV	TSVD-GCV	TR-DP	DSVD-DP
ϵ_{∞}	0.0043	0.0018	0.0105	0.0659
ϵ_2	0.0107	0.0083	0.0288	0.2016

Table 2: Generate g_1 from direct problem—relative root mean square errors under different regularization methods with 1% noise level

5. Suggested test 3: $g_1, u|_{\partial\Omega\setminus\Gamma} \to g_0$

In some applications, it is necessary to specify the flux g_1 on the Cauchy boundary. For example, the formulation in [12] requires $g_1 = 0$. In such cases, we first consider a direct problem with the mixed boundary conditions: $g_1|_{\Gamma} =$ 0 as required and assign some arbitrary values to u on $\partial \Omega \setminus \Gamma$. For direct problems of this type, the solution usually contains boundary singularities.

We take the top boundary of $\Omega = (-1, 1)^2$ as the Cauchy boundary Γ . To construct a numerical test, we solve the direct problem with u = xon Γ and $\partial_{\nu}u = 0$ for the remaining. We apply the FEM to solve the direct problem and use its solution value to define the Cauchy data g_0 at Γ . All four recommended regularization techniques in [17] are tested. Figure 3 shows approximations obtained by the MFS with different regularization techniques under 1% noise. All four solutions yields relative errors at around 5%. Although GCV seems to work better than LC in Figure 3, it is too preliminary to jump to this conclusion—it is not the interest of this work to perform extensive comparisons.

Solutions having singularities right at the boundary-singularities is actually not a very bad thing. If the solution has a singularity in which the boundary is smooth, *even for direct problems*, one must be careful when the MFS is applied—it is common to observe the Gibbs phenomenon near the point where the type of boundary condition changes [18].

In the last example, let Ω be the unit circle. We assign x^2y^3 to the missing upper-half boundary $\partial \Omega \setminus \Gamma$ and use zero Neumann boundary condition $g_1 =$ 0 on lower-half Γ to set up the direct problem. Going through all steps as described above, we obtain our test problem for the Cauchy problem (1). Unfortunately, none of the regularization techniques works well with the MFS approach—even if the data is noise-free (but still contains the numerical error from the FEM). This is exactly the type of experiments for testing the effectiveness of any forthcoming numerical methods.

6. Conclusion

In this short article, we pointed out that there exist some test examples whose Neumann boundary data are redundant and may not be suitable for evaluating (i.e. accuracy and robustness of) a numerical method. We provide an argument to show that, *in some cases*, the Dirichlet boundary condition on part of a circular domain can be extended to the whole. Hence,



(c) DSVD-LC (d) DSVD-GCV

Figure 3: Generate g_0 from direct problem—numerical solution yields from different regularization methods with 1% noise level.

the Neumann boundary data in the Cauchy problems is *theoretically* redundant. The key message to emphasize is to avoid drawing conclusion solely based on some overdetermined test problems. We suggest that a good set numerical examples should cover a wide varieties instead of examples with *numerically* redundancy only. A few different approaches for constructing numerical experiments are suggested.

In [17], it is suggested that using TR or DSVD with parameters selected by GCV or LC works well with the MFS in solving Cauchy problems of elliptic types. With the additional experiments in this paper, we have numerical evidences to support their conclusion. However, we also have examples, in which the Cauchy solution contains boundary singularities, such that all the MFS-related approaches in [17] fail.

Appendix

Acronyms and abbreviations

TR: Tikhonov Regularization

DSVD: Damped Singular Value Decomposition

TSVD: Truncated Singular Value Decomposition

LC: L-curve Criterion

GCV: Generalized Cross-Validation

DP: Discrepancy Principle

FEM: Finite Element Method

MFS: Method of Fundamental Solution

Setup Details

All domains are generated by a polar function r such that $\Omega = \{(r, \theta) : r < r(\theta), 0 \le \theta < 2\pi\}$. Consider the polar function r fixed thereafter. For some user-defined source distance d_s , we evenly place n_s source points on the fictitious boundary $\{(r, \theta) : r = r(\theta) + d_s, 0 \le \theta < 2\pi\}$. The Cauchy boundary is specified by an interval $\theta_{\Gamma} = [\theta_0, \theta_1]$ such that $\Gamma = \{(r, \theta) : r \le 1, r\}$.

 $r = r(\theta), \theta_0 \leq \theta \leq \theta_1$. Both Dirichlet and Neumann Cauchy data is, respectively collocated at m_D and m_N at evenly placed points on Γ . The number of evaluation points is always N = 1000 for finding numerical errors. Readers are referred to [17] for the details of MFS formulation and other regularization techniques.

- Figure 1(a) and 2(a): $\mathcal{L} = \Delta$, $r(\theta) = 1$, $n_s = 51$, $d_s = 10$, $\theta_{\Gamma} = [0, \pi]$, $m_D = 51$, $m_N = 0$.
- Figure 1(b) and 2(b): $\mathcal{L} = \Delta$, $r(\theta) = 1/\max(|\sin(\theta)|, |\cos(\theta)|), n_s = 51, d_s = 10, \theta_{\Gamma} = [0, \pi], m_D = 51, m_N = 0.$
- Section 3: $\mathcal{L} = \triangle$, $r(\theta) = 1$, $n_s = 102$, $d_s = 10$, $\theta_{\Gamma} = [\pi, 2\pi]$, $m_D = 51$, $m_N = 51$.
- Section 4 Direct: $\mathcal{L} = \Delta$, $r(\theta) = 1$, $n_s = 100$, $d_s = 5$, $\theta_{\Gamma} = [0, 2\pi]$, $m_D = 100$, $m_N = 0$.
- Section 4 Inverse: $\mathcal{L} = \Delta$, $r(\theta) = 1$, $n_s = 102$, $d_s = 10$, $\theta_{\Gamma} = [\pi, 2\pi]$, $m_D = 51$, $m_N = 51$.
- Section 5 Square: $\mathcal{L} = \Delta$, $r(\theta) = 1/\max(|\sin(\theta)|, |\cos(\theta)|)$, $n_s = 84$, $d_s = 10$, $\theta_{\Gamma} = [3\pi/4, 9\pi/4]$, $m_D = 42$, $m_N = 42$.
- Section 5 Circle: $\mathcal{L} = \Delta$, $r(\theta) = 1$, $n_s = 108$, $d_s = 10$, $\theta_{\Gamma} = [\pi, 2\pi]$, $m_D = 54$, $m_N = 54$.

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